Contents of Volume 15

NUMBER 1, 1 JANUARY 1988

Location of Double Bonds in Polyenic Long-chain Carboxylic Acids Containing a Conjugated Diene Unit 1
G. JANSSEN, A. VERHULST AND G. PARMENTIER

Collisional Spectroscopy as a Screening Procedure for the Determination of 2-(2-Furoyl)-4(5)-(2-Furanyl)-1H-Imidazole from Acid Hydrolysis of B-poly(L-Lysine) and B-Albumin 7
B. PELLI, A. STURARO, P. TRALDI, A. LAPOLLA, T. POLI, D. FEDELE AND G. CREPALDI

Mass Spectral Investigations on Trichothecene Mycotoxins IV—Collisionally Activated Dissociation Mass Spectra (Negative Ion) of Some Macrocyclic Trichothecenes 13
T. KRISHNAMURTHY AND E. W. SARVER

Rapid Quantification of 11 Prostanoids by Combined Capillary Column Gas Chromatography and Negative Ion Chemical Ionization Mass Spectrometry: Application to Prostanoids Released from Normal Human Embryonic Lung Fibroblasts in WI38 in a Culture Medium 25
N. SHINDO, T. SAITO AND K. MURAYAMA

Chemical Modification in Mass Spectrometry IV—2-Alkenyl-4,4-Dimethyloxazolines as Derivatives for the Double Bond Location of Longchain Olefinic Acids 33
J. Y. ZHANG, Q. T. YU, B. N. LIU AND Z. H. HUANG

A Gas Chromatographic/Mass Spectrometric Screening, Confirmation, and Quantification Method for Estrogenic Compounds 45
T. R. COVEY, D. SILVESTRE, M. K. HOFFMAN AND J. D. HENION

Measurement of Urinary Lactic, 3-Hydroxybutyric, Pyruvic and Acetoacetic Acids in a Single Anaysis Using Selected Ion Monitoring and Stable Isotope Labelling Techniques 57
O. A. MAMMER

NUMBER 2, 15 JANUARY 1988

Stereoselectivity of the 4-Hydroxylation of Debrisoquine in Man, Detected by Gas Chromatography/Mass Spectrometry 63
C. O. MEESE, C. FISCHER AND M. EICHELBAUM

Quantitative Determination of Arsenocholine and Acetylarsenocholine in Aquatic Organisms using Pyrolysis and Gas Chromatography/Mass Spectrometry 67
A. CHRISTAKOPOULOS, B. HAMASUR, H. NORIN AND I. NORDGREN

Linked Scan Investigation of Peptide Degradation Initiated by Liquid Secondary Ion Mass Spectrometry 79
R. KOSTIAINEN AND A. HESSO

Fast Atom Bombardment and Tandem Mass Spectrometry for Structure Determination: Remote Site Fragmentation of Steroid Conjugates and Bile Salts 89
K. B. TOMER AND M. L. GROSS

Evaluation of the Quantitative Analysis of a Steroid Sulphate using Fast Atom Bombardment and Tandem Mass Spectrometry 99
S. J. GASKELL

Packed Column Supercritical Fluid Chromatography/Mass Spectrometry using a Thermospray Source in the Filament-on-Mode 105
A. J. BERRY, D. E. GAMES, I. C. MYLCHREEST, J. R. PERKINS AND S. PLEASANCE

The Application of Gas Chromatographic/Mass Spectrometric Techniques to Spin Trapping. Conversion of α-Phenyl*N*-*tert*-Butyl Nitrone (PBN) Spin Adducts to Stable Trimethylsilylated Derivatives 111
E. G. JANZEN, P. H. KRYGSMAN AND D. L. HAIRE

***In vivo* Mwetabolism of (+)-*trans*-Delta-9-Tetrahydrocannabinol in the Mouse** 117
D. J. HARVEY

NUMBER 3, 1 FEBRUARY 1988

The Identification of Biologically Important Thiols 123
E. J. BREAUX, J. E. PATANELLA, E. F. SANDERS AND H. FUJIWARA

Gas Chromatography/Mass Spectrometry and Gas Chromatography/Tandem Mass Spectrometry of Methyl Ester/Methoxime/Trimethylsilyl Ether Derivatives of Prostaglandins 129
H. SCHWEER, H. W. SEYBERTH AND C. O. MEESE

Gas Chromatography/Mass Spectrometry and Gas Chromatography/Mass Spectrometry/Mass Spectrometry of Methyl Ester/Methoxime/Trimethylsilyl Ether Derivatives of Thromboxanes 139
H. SCHWEER, H. W. SEYBERTH, C. O. MEESE AND O. FÜRST

Negative Ion Chemical Ionization Gas Chromatography/Mass Spectrometry and Gas Chromatography/Tandem Mass Spectrometry of Prostanoid Pentafluorobenzyl Ester/Methoxime/Trimethylsilyl Ether Derivatives 143
H. SCHWEER, H. W. SEYBERTH, C. O. MEESE AND O. FÜRST

Determination of Sodium Salts of Monensins A and B in the Premix and the Fermentation Broth by Electron Impact Mass Spectrometry 153
M. BERAN, J. ZIMA AND V. SCHÖN

A Gas Chromatographic/Mass Spectrometric Assay for Catechol Estrogens in Microsomal Incubations: Comparison with a Radiometric Assay 157
D. J. PORUBEK AND S. D. NELSON

A Mass Spectral Study of Cyclophosphamide Concerning a Thermally Induced Rearrangement Reaction 163
E. BUSKER, E. KOBERSTEIN, U. NIEMEYER, J. ENGEL AND M. LINSCHEID

Electron Capture Negative Ion Chemical Ionization Analysis of Arachidonic Acid 175
J. S. HADLEY, A. FRADIN AND R. C. MURPHY

Continuous Flow Fast Atom Bombardment Liquid Chromatography/Mass Spectrometry: Studies Involving Conventional Bore Liquid Chromatography with Simultaneous Ultraviolet Detection 179
D. E. GAMES, S. PLEASANCE, E. D. RAMSEY AND M. A. McDOWALL

Book Reviews 183

NUMBER 4, 15 FEBRUARY 1988

Mass Spectral Investigations on Trichothecene Mycotoxins. V. Direct Analysis of Satratoxins by Tandem Mass Spectrometric Techniques 185
T. KRISHNAMURTHY AND E. W. SARVER

Rapid Identification of Drug Metabolites with Tandem Mass Spectrometry 193
M. S. LEE AND R. A. YOST

Identification of Metabolites of Tiropramide in Human Urine 205
R. ARIGONI, R. CHISTÈ, F. MAKOVEC, I. SETNIKAR, E. BENFENATI AND R. FANELLI

Mass Spectral Analysis of some Derivatives and *in vitro* Metabolites of Steviol, the Aglycone of the Natural Sweeteners, Stevioside, Rebaudioside A, and Rubusoside 211
C. M. COMPADRE, R. A. HUSSAIN, N. P. D. NANAYAKKARA, J. M. PEZZUTO AND A. D. KINGHORN

Thermospray Liquid Chromatography Tandem Mass Spectrometry: Application to the Elucidation of Zolpidem Metabolism 223
S. VAJTA, J. P. THENOT, F. de MAACK, G. DEVANT AND M. LESIEUR

Mass Spectrometric Characterization of Some Human Metabolites of Flumecinol 157
J. TAMÁS, M. MÁK, I. KLEBOVICH, L. VERECZKEY AND E. TÓTH

Positive Ion Fast Atom Bombardment Mass Spectrometry of Reductively Pyridylaminated Maltooligosaccharides and its Application to α-Amylase Assay 233
S. HONDA, K. KAKEHI, T. OHMURA AND M. MORITA

Short Communication

Chemical Ionization Mass Spectra of High Molecular Weight, Biologically Active Compounds Produced Following Supercritical Fluid Chromatography 239
H. T. KALINOSKI, B. W. WRIGHT AND R. D. SMITH

NUMBER 5, 1 MARCH 1988

Synthesis of Deuterium-labelled Elliptinium and its Use in Metabolic Studies 243
A. GOUYETTE

Determination of Melatonin in Blood Plasma, Using Capillary Gas Chromatography and Electron Impact Medium-Resolution Mass Spectrometry 249
C. R. LEE AND H. ESNAUD

Comparison of Methanol Thermospray (Filament On) and Direct Chemical Ionization Mass Spectrometry to the Study of Biologically Active Steroids 253
P. R. DAS, B. N. PRAMANIK, R. D. MALCHOW AND K. J. NG

Fast Atom Bombardment Mass Spectrometry of High-Molecular-Weight Fraction of Porphyrin-based Photodynamic Therapy Drugs 257
B. MUSSELMAN, D. KESSEL AND C. K. CHANG

Determination of Pyrrolizidine Alkaloid Metabolites from Mouse Liver Microsomes using Tandem Mass Spectrometry and Gas Chromatography/Mass Spectrometry 265
C. K. WINTER, H. J. SEGALL AND A. D. JONES

Identification and Quantification of Halogenated and Non-halogenated Octylphenol Polyethoxylate Residues by Gas Chromatography/Mass Spectrometry using Electron Ionization and Chemical Ionization 275
E. STEPHANOU, M. REINHARD AND H. A. BALL

Determination of Boldenone Sulfoconjugate and Related Steroid Sulfates in Equine Urine by High-performance Liquid Chromatography/Tandem Mass Spectrometry 283
L. O. G. WEIDOLF, E. D. LEE AND J. D. HENION

(^{18}O) Quinolinic Acid: Its Esterification without Back Exchange for Use as Internal Standard in the Quantification of Brain and CSF Quinolinic Acid 291
M. P. HEYES AND S. P. MARKEY

Laser Desorption/Fourier Transform Ion Cyclotron Resource Mass Spectrometry: Digoxin, Digitoxin, and their Reduced and Sugar-hydrolyzed Metabolites 117
R. E. SHOMO, II., A. CHANDRASEKARAN, A. G. MARSHALL, R. H. REUNING AND L. W. ROBERTSON

Forthcoming Events 303

NUMBER 6, 15 MARCH 1988

^{252}CF Plasma Desorption Mass Spectometry of a Polycyclic Peptide Antibiotic, Nisin 305
P. ROEPSTORFF, P. F. NIELSEN, I. KAMENSKY, A. G. CRAIG AND R. SELF

Automated Profiling of Urinary Organic Acids by Dual-column Gas Chromatography and Gas Chromatography/Mass Spectrometry 311
M. F. LEFEVERE, B. J. VERHAEGHE, D. M. DECLERCK AND A. P. DE LEENHEER

Identification of a Biliary Metabolite of Cisapride 323
W. LAUWERS, L. LE JEUNE AND W. MEULDERMANS

Conjugation Reactions of Polyaromatic Quinones to Mono- and Bisglutathionyl Adducts: Direct Analysis by Fast Atom Bombardment Mass Spectrometry 329
M. HEIDMANN, P. FONROBERT, M. PRZYBYLSKI, K. L. PLATT, A. SEIDEL AND F. OESCH

An Efficient Algorithm for Sequencing Peptides using Fast Atom Bombardment Mass Spectral Data 333
M. M. SIEGEL AND N. BAUMAN

The Enzymatic and Mass Spectrometric Identification of 2-Oxophytanic Acid, a Product of the Peroxisomal Oxidation of L-2-Hydroxyphytanic Acid 345
J. VAMECQ AND J.-P. DRAYE

SHORT COMMUNICATION
Collisional Spectroscopy in Structural Characterization of Melanins 2—Laser Desorption Experiments on Bio- and Synthetic Tryptophan Melanins 353
G. ALLEGRI, M. BIASIOLO, G. FRISON, B. PELLI AND P. TRALDI

Book Reviews 357

NUMBER 7, 1 APRIL 1988

Constituents of *Justice pectoralis* Jacq. 2. Gas Chromatography/Mass Spectrometry of Simple Coumarins, 3-Phenylpropionic Acids and their Hydroxy and Methoxy Derivatives 413
J. X. DE VRIES, B. TAUSCHER AND G. WURZEL

A Study of the Positive and Negative Ion Fast Atom Bombardment Mass Spectra of α-Amino Acids 419
W. KULIK AND W. HEERMA

Ion Chemistry of a Gas Chromatographic/Mass Spectrometric Ion Abundance Calibrant 429
Y. TONDEUR, W. J. NIEDERHUT, J. E. CAMPANA, R. K. MITCHUM, G. W. SOVOCOOL AND J. R. DONNELLY

Direct Stereochemical Assignment of Sugar Subunits in Naturally Occurring Glycosides by Low Energy Collision Induced Dissociation. Application to Papulacandin Antibiotics 441
D. R. MUELLER, B. M. DOMON, W. BLUM, F. RASCHDORF AND W. J. RICHTER

Measurement of ^{13}C-Glucose Oxidation Rate Using Mass Spectrometric Determination of the CO_2:Ar Ratio and Spirometry 447
Y. GHOOS, P. RUTGEERTS, G. VANTRAPPEN AND M. HIELE

Gas Chromatographic/Mass Spectrometric Identification of Chlorinated and Oxygenated Cyclohexene Artifacts Formed during the Analysis of Chlorinated Water Samples 453
A. M. DIETRICH, R. F. CHRISTMAN AND G. S. DURELL

Short Communications

Bacteriophage Edoglycanases and Desorption Chemical Ionization Mass Spectrometry (DCI–MS) to Sequence Bacterial Antigens 459
G. G. S. DUTTON, G. EIGENDORF, Z. LAM AND A. V. S. LIM

Analysis of Middle Mass Peptides by Thermospray LC/MS 461
R. J. RUDEWICZ

Letter to the Editor 465

Book Review 465

NUMBER 8, 15 APRIL 1988

Constituents of *Justicia pectoralis* Jacq. 2. Gas Chromatography/Mass Spectrometry of Simple Coumarins, 3-Phenylpropionic Acids and their Hydroxy and Methoxy Derivatives 413
J. X. DE VRIES, B. TAUSCHER AND G. WURZEL

A Study of the Positive and Negative Ion Fast Atom Bombardment Mass Spectra of α-Amino Acids 419
W. KULIK AND W. HEERMA

Ion Chemistry of a Gas Chromatographic/Mass Spectrometric Ion Abundance Calibrant 429
Y. TONDEUR, W. J. NIEDERHUT, J. E. CAMPANA, R. K. MITCHUM, G. W. SOVOCOOL AND J. R. DONNELLY

Direct Stereochemical Assignment of Sugar Subunits in Naturally Occurring Glycosides by Low Energy Collision Induced Dissociation. Application to Papulacandin Antibiotics 441
D. R. MUELLER, B. M. DOMON, W. BLUM, F. RASCHDORF AND W. J. RICHTER

Measurement of $_{13}$C-Glucose Oxidation Rate Using Mass Spectrometric Determination of the CO_2:Ar Ratio and Spirometry 447
Y. GHOOS, P. RUTGEERTS, G. VANTRAPPEN AND M. HIELE

Gas Chromatographic/Mass Spectrometric Identification of Chlorinated and Oxygenated Cyclohexene Artifacts Formed during the Analysis of Chlorinated Water Samples 453
A. M. DIETRICH, R. F. CHRISTMAN AND G. S. DURELL

Short Communications

Bacteriophage Endoglycanases and Desorption Chemical Ionization Mass Spectrometry (DCI-MS) to Sequence Bacterial Antigens 459
G. G. S. DUTTON, G. EIGENDORF, Z. LAM AND A. V. S. LIM

Analysis of Middle Mass Peptides by Thermospray LC/MS 461
P. J. RUDEWICZ

Letter to the Editor 465

Book Review 465

NUMBER 9, 1 MAY 1988

The Applicability of Evacuated Serological Tubes for the Collection of Breath for Isotopic Analysis of CO_2 by Isotope Ratio MAss Spectrometry 467
E. MILNE AND B. A. McGAW

Calculation of the Relative Frequencies of Stable Isotope Labelled and Unlabelled Molecules in a Gas Chromatographic Peak Using Gas Chromatography/Mass Spectrometry 473
R. H. DUNSTAN

The Quantification of Synthetic Corticosteroids Using Isotope Dilution Gas Chromatography Negative Chemical Ionization Mass Spectrometry 479
J. M. MIDGLEY, D. G. WATSON, T. HEALEY AND M. NOBLE

Mass Spectral Characteristics of Derivatized Metabolites of Benzo[*A*]Pyrene 485
E. K. CHESS, B. L. THOMAS, D. J. HENDREN AND R. M. BEAN

'Revised' Mass Spectral Identification of 2-Amino-4-(5-nitro-2-furyl) Thiazole Metabolites 495
M. B. MATTAMMAL, V. M. LAKSHMI, T. V. ZENSER, R. B. DAVIS AND E. WHITE V

Characterization of Doxylamine and Pyrilamine Metabolites via Thermospray/Mass Spectrometry and Tandem Mass Spectrometry 501
W. A. KORFMACHER, C. L. HOLDER, L. D. BETOWSKI AND R. K. MITCHUM

Leukotriene Biosynthesis: Direct Chemical Ionization Mass Spectrometry of Underivatized Arachidonic Acid Metabolites 509
J. GUT, J. R. TRUDELL AND G. C. JAMIESON

Short Communication
Analysis of the Polycyclic Aromatic Compounds of Diesel Fuel by Gas Chromatography with Ion-trap Detection 517
P. T. WILLIAMS, G. E. ANDREWS, K. D. BARTLE, P. BISHOP AND P. WATKINS

NUMBER 10, 15 MAY 1988

A Rapid and Sensitive Method for the Determination of γ-Hydroxybutyric Acid and *trans*-γ-Hydroxycrotonic Acid in Rat Brain Tissue by Gas Chromatography/Mass Spectrometry with Negative Ion Detection 521
J. D. EHRHARDT, Ph. VAYER AND M. MAITRE

Negative Ion Mass Spectra of Dihydropyridine Calcium-channel Blockers 525
J. D. EHRHARDT AND J. M. ZIEGLER

Self-chemical Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: Identification and Characterization of Modified and Unmodified Bases and Nucleosides 529
R. R. WELLER, J. A. MAYERNIK AND C. S. GIAM

An Extraction-derivatization Method Suitable for the Analysis of Biogenic Amines by Gas Chromatography Negative Ion Mass Spectrometry 535
J. M. MIDGLEY, J. MACLACHLAN AND D. G. WATSON

A Determination of the Positions of Disulphide Bonds in Paim I, α-Amylase Inhibitor from *Streptomyces corchorushii*, Using Fast Atom Bombardment Mass Spectrometry 541
S. AKASHI, K. HIRAYAMA, T. SEINO, S.-I. OZAWA, K.-I. FUKUHARA, N. OOUCHI, A. MURAI, M. ARAI, S. MURAO, K. TANAKA AND I. NOJIMA

Analysis of Sub-microgram Quantities of Nucleotides by Fast Atom Bombardment Mass Spectrometry 547
H. MOSER AND G. W. WOOD

Capillary Column Isobutane Chemical Ionization Mass Spectrometry of Mustard and Related Compounds 553
P. A. D'AGOSTINO AND L. R. PROVOST

A Selected Ion Monitoring Assay for Tributyltin and Its Degradation Products 565
J. GREAVES AND M. A. UNGER

Nucleophilic Reactions Between Biological Conjugates and Tetraalkylammonium Ion Pair Reagents During Desorption Chemical Ionization 571
W. B. EMARY, Z. SHEN, R. G. COOKS, I. PLAKUNOV AND W. M. BAIRD

Short Communication

Constant Neutral Loss Spectra of Small Peptides 577
E. DE PAUW, G. PELZER AND K. NASAR

NUMBER 11, 1 JUNE 1988

Use of Ion-Molecule Reactions for Selected Reaction Monitoring in Gas Chromatographic/Tandem Mass Spectrometric Analyses in Two Model Systems 583
M. T. KINTER AND M. M. BURSEY

Identification of Flavonoid Glycosides Isolated from Plants by Fast Atom Bombardment Mass Spectrometry and Gas Chromatography/Mass Spectrometry 589
M. STOBIECKI, W. OLECHNOWICZ-STĘPIEŃ, H. RZĄDKOWSKA-BODALSKA, W. CISOWSKI AND E. BUDKO

A Rapid Method for the Structural Characterization of Sulphated Phlorotannins by Negative Ion Fast Atom Bombardment Mass Spectrometry and Acetylation on the Target 595
J. PETER-KATALINIĆ, H. EGGE, B. DEUTSCHER, W. KNÖß AND K.-W. GLOMBITZA

Stable Isotope Dilution Method using Thermospray Liquid Chromatography/Mass Spectrometry for Quantification of Daily Cortisol Production in Humans 603
N. V. ESTEBAN, A. L. YERGEY, D. J. LIBERATO, T. LOUGHLIN AND D. L. LORIAUX

Laser Desorption/Fourier Transform Mass Spectrometry of Steroids 609
E. T. FUNG AND C. L. WILKINS

Characterization of Glutathione Conjugates by Fast Atom Bombardment/Tandem Mass Spectrometry 615
P. E. HAROLDSEN, M. H. REILLY, H. HUGHES, S. J. GASKELL AND C. J. PORTER

Analysis of Glutathione Conjugates and Related Compounds by Thermospray Mass Spectrometry 623
C. E. PARKER, J. S. M. DE WIT, R. W. SMITH, M. B. GOPINATHAN, O. HERNANDEZ, K. B. TOMER, C. H. VESTAL, J. M. SANDERS AND J. R. BEND

Errata 635

NUMBER 12, 15 JUNE 1988

The Use of Alkoxycarbonyl Derivatives for the Mass Spectral Analysis of Drug-Thioether Metabolites. Studies with the Cysteine, Mercapturic Acid and Glutathione Conjugates of Acetaminophen 637
K.-J. HOFFMANN AND T. A. BAILLIE

FAB and Tandem Mass Spectrometry for Endorphin- and ACTH Peptides of Molecular Weight to 2000 649
K. B. TOMER, M. L. GROSS, H. ZAPPEY, R. H. FOKKENS AND N. M. M. NIBBERING

A Systematic Study of Instrumental Parameters Affecting Electron Capture Negative Ion Mass Spectra 659
E. A. STEMMLER AND R. A. HITES

Bromo- and Bromochloro-polynuclear Aromatic Hydrocarbons, Dioxins and Dibenzofurans in Municipal Incinerator Fly Ash 669
G. W. SOVOCOOL, R. K. MITCHUM, Y. TONDEUR, W. D. MUNSLOW, T. L. VONNAHME AND J. R. DONNELLY

Short Communications

Determination of Melatonin by GC–MS: Problems with Solid Phase Extraction (SPE) Columns 677
C. R. LEE AND H. ESNAUD

Fast Atom Bombardment Mass Spectrometry of Protected Peptide Segments 681
A. GRANDAS, E. PEDROSO, A. FIGUERAS, J. RIVERA AND E. GIRALT

Forthcoming Events 685